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A BOLTZMANN TRANSPORT CODE FOR ION PENETRATION IN MATTER.(U)

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A Boltzmann Transport Code for Ion Penetration in Matter

G. P. Mueller and Mervine Rosen

Radiation-Matter Interactions Branch
Radiation Technology Division

July 1977

NAVAL RESEARCH LABORATORY
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The Boltzmann equation for the single particle distribution function for a heavy ion beam penetrating matter is solved. We assume rotational and translational invariance, plane symmetry and time independence. A Hermite and Legendre polynomial expansion of the distribution function is made in the configuration and angular coordinates, respectively. A code for numerically solving the integral equations for the energy dependent expansion coefficients has been written and solved explicitly for the case of a monoenergetic 200 keV beam of antimony ions incident on germanium. The range distribution of stopped Sb ions and the distribution of energy loss from the beam are presented.

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CONTENTS

A BOLTZMANN TRANSPORT CODE FOR ION PENETRATION IN MATTER

A. Introduction

Boltzmann transport theory has been thoroughly investigated for cases where specific physical assumptions - isotropic elastic scattering cross sections in the center of mass frame (slow neutron transport) or small angle elastic scattering (passage of high energy particles through matter) - allow drastic mathematical simplifications. No such simplifying conditions exist when one is considering either low energy ions, which come to rest in the bombarded material, or the recoils they produce in elastic collisions with target atoms. However, the single particle distribution functions for the penetrating ions and the recoil atoms contain a great deal of information, which may be used, e.g., to calculate directly range distributions of both beam and recoil atoms, energy and damage distributions in the bombarded material and to study ion implantation and sputtering phenomena. I. Manning and D. W. Padgett[1] (hereafter referred to as MP) have developed a formalism for describing the penetration of amorphous matter by a heavy ion beam which is based on the Boltzmann transport equation and uses Lindhard atomic collision cross sections. This formalism was later extended by Mueller[2] to include inelastic losses.

Note: Manuscript submitted July 6, 1977.

In this paper, a method in which the single particle distribution function is expanded in Hermite and Legendre polynomials is described and applied to the implementation of the Manning-Padgett heavy ion transport formalism. By way of a demonstration calculation we have considered a beam of 200 keV antimony ions incident on germanium. This particular case was chosen because it seems typical for a class of applications we have in mind, and because experimental data[3] and theoretical calculations[4] of energy deposition are already available here.

As discussed in MP, most of the calculations of ion penetration have heretofore been based on transport theories of the Lindhard type,[5,6,7] whereas the transport theory we deal with is based on the Boltzmann transport equation.

B. Form of the Solution

Consider the Boltzmann equation for the vector flux Ψ of the incident beam, under the simplifying assumptions of rotational invariance, translational invariance, plane symmetry and time independence:[8]

$$\mu \frac{\partial}{\partial x} \Psi(E,x,\mu) + N\sigma^T(E)\Psi(E,x,\mu) - \frac{\partial}{\partial E} (S(E)\Psi(E,x,\mu)) = \mathscr{S}(E,x,\mu) + N\mu v \int d^3v'(\mu'v')^{-1}\sigma(\underset{\sim}{v}' \rightarrow \underset{\sim}{v})\Psi(E',x,\mu'), \quad (1)$$

where x is the distance along the direction of the bombarding beam and perpendicular to the target surface, v is the ion velocity, N is the density of target atoms,

$$E = \tfrac{1}{2} m v^2 \tag{2}$$

$$\mu = \hat{v} \cdot \hat{x} \ . \tag{3}$$

S(E) is the inelastic stopping power (we take inelastic electronic energy losses into account in the continuous slowing down approximation), $\mathcal{S}$ is the source term of the beam ion flux, and

$$\Psi(E,x,\mu) = \mu \, v \, N(E,x,\mu) \ , \tag{4}$$

with

$$N(E,x,\mu)\, dE\, dx\, d\mu = \text{number of beam ions with energy in the interval } dE \text{ about } E, \text{ direction cosine } d\mu \text{ about } \mu, \text{ and at distance } dx \text{ about } x; \tag{5}$$

and the elastic binary collision cross section is defined such that

$$N \sigma(\underset{\sim}{v}' \to \underset{\sim}{v})\, v' \,\Psi(\underset{\sim}{r},\underset{\sim}{v}',t)\, d^3v'\, d^3r\, dt$$

= the probable number of beam particles with velocity in d^3v' about $\underset{\sim}{v}'$, located in d^3r about $\underset{\sim}{r}$, which undergo a collision in time dt about t such that their final velocities lie in d^3v about $\underset{\sim}{v}$. (6)

The total elastic cross section, $\sigma^T(E)$, is given by

$$\sigma^T(E) = \int d^3v' \sigma(\overline{v} \to \overline{v}') \ . \tag{7}$$

It should be stressed that our transport approach models the target as being amorphous.

We employ the boundary condition used by Winterbon, Sigmund and Sanders (WSS) in their work[7] and model the target as being infinite in every direction; over the entire $x = 0$ plane there is embedded in the target a source of monoenergetic atoms, all traveling in the positive x direction. This boundary condition represents an actual ion bombardment only to the extent that scatterings back and forth through the $x = 0$ plane can be neglected. For the case of our demonstration calculation, there should be a negligible number of such scatterings.

We note however that our approach nevertheless differs to a considerable extent from that of WSS. The WSS distribution $F(\underset{\sim}{r},\underset{\sim}{v})$ is a distribution of deposited energy, whereas ours is the distribution in energy and angle of the beam ions as they traverse the target. In addition, WSS solve for moments of their distribution from which they must reconstruct the distribution, whereas we solve directly for the distribution by an expansion in Hermite and Legendre polynomials with energy dependent parameters built into the expansion functions. The use of these energy dependent functions, $\overline{x}(E)$ and $\xi(E)$ (see next section), allows us great flexibility in improving the convergence of the expansion. Given $\Psi(E,x,\mu)$, we are able to calculate with relative ease the distribution of deposited energy, the energy dependent spatial distribution of beam ions and moments of these distributions.

A method of handling the singularities near the boundary surface is presented in references 1 and 2. As is done there the solution for the vector flux is written in the form

$$\Psi = \Psi_0 + \Psi_1 + \Psi_2 + \Phi . \tag{8}$$

The terms Ψ_0, Ψ_1 and Ψ_2 represent the vector flux of particles which have undergone, respectively, zero, one and two elastic collisions with target atoms. The Φ term represents particles which have undergone three or more elastic collisions.

All of our results are normalized to unit incoming flux. We write the source term in the Boltzmann equation for the incoming ions in the form

$$\mathscr{S}(E,x,\mu) = 4\delta(x)\delta(\mu - 1)\delta(E - E_B) \ , \tag{9}$$

where E_B is the incident beam energy.

For convenience we rewrite Eq. (8) so as to exhibit explicitly the singularities arising from the source term.

$$\begin{aligned} \Psi(E,x,\mu) &= \delta(\mu - 1)\delta(E - E_B)\psi_0(x) \\ &+ \delta(\mu - g(E_B,E))\psi_1(E,x) \\ &+ \Psi_2(E,x,\mu) \\ &+ \Phi(E,x,\mu) \ , \end{aligned} \tag{10}$$

where $g(E_B,E)$ is the cosine of the scattering angle in the laboratory system for a beam ion entering with energy E_B and exiting with energy E. The first three contributions are solved for explicitly, and the problem is reduced to solving for Φ, which is by far the most important portion of Ψ, but contains neither the singularities of the Ψ_0 and Ψ_1 terms nor the extremely peaked behavior that Ψ_2 exhibits.[9]

C. Explicit Expressions for Ψ_0, Ψ_1, and Ψ_2

It is convenient to define a number of quantities here which appear frequently in many expressions that follow. For an elastic scattering, corresponding to $\underset{\sim}{v}' \to \underset{\sim}{v}$ (where both $\underset{\sim}{v}'$ and $\underset{\sim}{v}$ refer to the beam ion), one obtains for the cosine of the scattering angle in the lab system

$$\hat{v}' \cdot \hat{v} = g(E',E) = \tfrac{1}{2}[(M + 1)(E/E')^{\frac{1}{2}} - (M - 1)(E'/E)^{\frac{1}{2}}] \tag{11}$$

where

$$M = A_2/A_1 \tag{12}$$

and A_1 and A_2 are the masses of the beam ions and target atoms, respectively. The cross section $\sigma(\underset{\sim}{v}' \to \underset{\sim}{v})$ of Eq. (6) can be written in the form

$$\sigma(v' \to v) = \frac{1}{2\pi}\,\delta(\hat{v} \cdot \hat{v}' - g(E',E))F(E',E) \; . \tag{13}$$

For convenience, we also define the quantity

$$\mathcal{F}(E',E) = (2/A_1{}^3)^{\frac{1}{2}} N E^{\frac{1}{2}} F(E',E) \; . \tag{14}$$

The total cross section corresponding to the differential cross section (13) is

$$N\sigma^T(E') = \int_{E'/\beta}^{E'} dE\,\mathcal{F}(E',E) \; , \tag{15}$$

where

$$\beta = \left(\frac{M + 1}{M - 1}\right)^2 \tag{16}$$

and E'/β is the minimum possible energy for an outgoing beam ion following an elastic collision. For later use, we also define the quantities

$$L(E,\mu) = N\sigma^T(E)/\mu \;, \tag{17}$$

$$\ell(E) = L(E,g(E_B,E)) = N\sigma^T(E)/g(E_B,E) \;, \tag{18}$$

$$\ell_B = \ell(E_B) = N\sigma^T(E_B) \;. \tag{19}$$

In evaluating Ψ_0, Ψ_1, and Ψ_2 we have neglected the contribution from inelastic electronic energy losses. As will be seen later (Fig. 1) this should have a negligible effect on the final solution. Inelastic losses were not neglected in the calculation of Φ. In deriving the equation below we assume the inelastic loss term in the Boltzmann equation to be absent. For the sake of clarity this is true also for the equations that determine Φ. In Appendix A, however, we show how those equations are modified to include the contribution of these losses.

When we substitute the solution (10) into the Boltzmann equation and use the limiting procedures of MP[1] to separate the various terms according to their singular behavior, we obtain the four equations

$$\frac{d}{dx}\,\psi_0(x) + N\sigma^T(E_B)\psi_0(x) = \delta(x) \;, \tag{20}$$

$$g(E_B,E)\,\frac{\partial}{\partial x}\,\psi_1(E,x) + N\sigma^T(E)\psi_1(E,x) \tag{21}$$

$$= g(E_B,E)\psi_0(x)\mathcal{F}(E_B,E) \;,$$

$$\mu\,\frac{\partial}{\partial x}\,\Psi_2(E,x,\mu) + N\sigma^T(E)\Psi_2(E,x,\mu) \tag{22}$$

$$= \frac{\mu}{2\pi}\int_E^{\beta E} dE'\mathcal{F}(E',E)\int d\hat{v}'\delta(\hat{v}\cdot\hat{v}' - g(E',E)) \times$$

$$\times \; \mu'^{-1}\delta(\mu' - g(E_B,E'))\Psi_1(E',x);$$

also

$$\mu \frac{\partial}{\partial x} \Phi(E,x,\mu) + N\sigma^T(E)\Phi(E,x,\mu) \tag{23}$$

$$= \frac{\mu}{2\pi}\int_E^{\beta E} dE'\mathcal{F}(E',E)\int d\hat{v}'\delta(\hat{v}\cdot\hat{v}' - g(E',E)) \times$$

$$\times \; \mu'^{-1}[\Psi_2(E',x,\mu') + \Phi(E',x,\mu')] .$$

Equation (20) is simply solved to yield

$$\Psi_o(x) = U(x)\exp\{-\ell_B x\} , \tag{24}$$

where U(x) is the unit step function. In solving for Ψ_1, we note that the mass ratio M in the case of antimony on germanium is such that the maximum scattering angle is approximately 36°. The cosine factor $g(E_B,E)$ in Eq. (21) can never be negative; in fact, three or more collisions are required before the kinematics allow a beam ion to be scattered to a backward direction.

As can be easily verified by substitution, the solution of Eq. (21) has the form

$$\Psi_1(E,x) = e^{-\ell(E)x}\int_{-\infty}^{x} dx' e^{\ell(E)x'}\Psi_o(x')\mathcal{F}(E_B,E) , \tag{25}$$

or

$$\Psi_1(E,x) = \mathcal{F}(E_B,E)T_1(\ell_B,\ell(E);x) , \tag{26}$$

where

$$T_1(a,b;x) = \frac{e^{-ax} - e^{-bx}}{b - a} U(x) . \tag{27}$$

Mass ratios that allow backward scattering in a single collision are handled just as simply, but the resulting expression for ψ_1 is slightly different.

By performing the angular integrals, Eq. (22) can be rewritten as

$$\mu \frac{\partial}{\partial x} \Psi_2(E,x,\mu) + N\sigma^T(E)\Psi_2(E,x,\mu)$$
$$= \frac{\mu}{\pi} \int_E^{\beta E} dE' \mathcal{F}(E',E)\psi_1(E',x) g^{-1}(E_B,E')\kappa^{-\frac{1}{2}} U(\kappa) , \tag{28}$$

where

$$\kappa = \kappa(E',E,\mu) = (\mu_+ - \mu)(\mu - \mu_-) \tag{29}$$

and

$$\mu_\pm = g(E_B,E')g(E',E) \pm \sqrt{1 - g^2(E_B,E')} \sqrt{1 - g^2(E',E)} . \tag{30}$$

As can again be verified by substitution, the solution of Eq. (28) is

$$\Psi_2(E,x,\mu) = \mu^{-1} e^{-L(E,\mu)x} \int_o^x dx' e^{L(E,\mu)x'} \frac{\mu}{\pi} \int_E^{\beta E} dE' \mathcal{F}(E',E)$$
$$\times \psi_1(E',x') g^{-1}(E_B,E')\kappa^{-\frac{1}{2}} U(\kappa) \tag{31}$$

$$= \frac{1}{\pi} \int_E^{\beta E} dE' \mathcal{F}(E',E)\mathcal{F}(E_B,E') g^{-1}(E_B,E')$$
$$\times \kappa^{-\frac{1}{2}} U(\kappa) T_2(\ell_B, \ell(E'), L(E,\mu);x) , \tag{32}$$

where

$$T_2(a,b,c;x) = \frac{1}{b-a}\left\{\frac{e^{-ax} - e^{-cx}}{c-a} - \frac{e^{-bx} - e^{-cx}}{c-b}\right\}. \tag{33}$$

After some manipulation, one can show that $K(E',E,\mu)$ can be written in the form

$$K(E',E,\mu) = \frac{(E_+ - E')(E' - E_-)}{E'} \; \frac{\mu_o + (M^2 - 1)\mu}{2\sqrt{EE_B}} , \tag{34}$$

where

$$\mu_o = \tfrac{1}{2}[(M+1)^2(E/E_B)^{\frac{1}{2}} + (M-1)^2(E_B/E)^{\frac{1}{2}}] \tag{35}$$

and

$$E_\pm = \frac{M^2 - \mu^2 + \mu\mu_o \pm (1-\mu^2)^{\frac{1}{2}}(M^4 - (\mu - \mu_o)^2)^{\frac{1}{2}}}{\mu_o + (M^2 - 1)\mu}(EE_B)^{\frac{1}{2}}. \tag{36}$$

We note that the minimum value of μ after two scatterings is given by

$$\mu_m = \mu_o - M^2. \tag{37}$$

The expression for Ψ_2 can now be written

$$\begin{aligned}\Psi_2(E,x,\mu) = {} & \frac{1}{\pi} U(x)U(\mu - \mu_m) \\ & \times \int_{E_-}^{E_+} dE' \mathcal{F}(E_B,E')\mathcal{F}(E',E)T_2(\ell_B,\ell(E'),L(E,\mu);x) \\ & \times [g(E_B,E')\sqrt{K(E',E,\mu}\,]^{-1}. \end{aligned} \tag{38}$$

D. The Hermite Polynomial Expansion of $\Phi(E,x,\mu)$

We solve Eq. (23) by expanding $\Phi(E,x,\mu)$ in Hermite polynomials in the variable x and Legendre polynomials in the variable μ. Starting with the Hermite expansion we write

$$\Phi(E,x,\mu) = \exp\left\{-\left(\frac{x - \bar{x}(E)}{\xi(E)}\right)^2\right\} \times \sum_{s=0}^{\infty} h_s^{-1} \varphi_s(E,\mu) H_s\left(\frac{x - \bar{x}(E)}{\xi(E)}\right) \tag{39}$$

and

$$\Psi_2(E,x,\mu) = \exp\left\{-\left(\frac{x - \bar{x}(E)}{\xi(E)}\right)^2\right\} \times \sum_{s=0}^{\infty} h_s^{-1} \Psi_{2;s}(E,\mu) H_s\left(\frac{x - \bar{x}(E)}{\xi(E)}\right), \tag{40}$$

where h_s is the normalizing factor

$$h_s = \sqrt{\pi}\, 2^s s! \tag{41}$$

arising from the integral

$$\int_{-\infty}^{\infty} dy\, e^{-y^2} H_s(y) H_n(y) = h_s \delta_{sn} . \tag{42}$$

We substitute the expansions (39) and (40) into Eq. (23), use the fact that

$$\frac{\partial}{\partial x}\left[e^{-\left\{\left(\frac{x - \bar{x}}{\xi}\right)^2\right\}} H_n\left(\frac{x - \bar{x}}{\xi}\right)\right] = -\xi^{-1} e^{-\left\{\left(\frac{x - \bar{x}}{\xi}\right)^2\right\}} H_{n+1}\left(\frac{x - \bar{x}}{\xi}\right) \tag{43}$$

and operate on both sides with

$$\int_{-\infty}^{\infty} dx \, \exp\left\{-\left(\frac{x - \overline{x}(E)}{\xi(E)}\right)^2\right\} H_n\left(\frac{x - \overline{x}(E)}{\xi(E)}\right)$$

and obtain

$$\begin{aligned} -2n\mu\varphi_{n-1}(E,\mu) &+ \xi(E)\, N\sigma^T(E)\varphi_n(E,\mu) \\ &= \frac{\mu}{2\pi}\int_E^{\beta E} dE'\,\mathcal{F}(E',E)\int_{-1}^{1} d\mu' \int_0^{2\pi} d\varphi' \mu'^{-1} \\ &\times \delta(\hat{v}\cdot\hat{v}' - g(E',E)) \\ &\times \sum_{s=0}^{n} Q_{n,s}(E',E)\,[\Psi_{2;s}(E',\mu') + \varphi_s(E',\mu')] \, , \end{aligned} \tag{44}$$

where

$$\begin{aligned} Q_{n,s}(E',E) &= h_s^{-1}\int_{-\infty}^{\infty} dx\, H_n\left(\frac{x - \overline{x}(E)}{\xi(E)}\right) \\ &\times \exp\left\{-\left(\frac{x - \overline{x}(E')}{\xi(E')}\right)^2\right\} H_s\left(\frac{x - \overline{x}(E')}{\xi(E')}\right). \end{aligned} \tag{45}$$

The evaluation of $Q_{n,s}(E',E)$ is left to Appendix B.

Henceforth, we will use the notation

$$\overline{x} = \overline{x}(E)\,,\; \xi = \xi(E)\,,\; \overline{x}' = \overline{x}(E')\,,\; \xi' = \xi(E')\,. \tag{46}$$

The functions $\overline{x}(E)$ and $\xi(E)$ are yet to be specified. The advantage of introducing $\overline{x}(E)$ and $\xi(E)$ is that much of the gross behavior (as a function of x) of the distribution function can be built into the

Gaussian factor in expansion (39). Consequently, many fewer terms should be required in the Hermite expansion than would be the case if we set

$$\bar{x}(E) = 0, \; \xi(E) = \text{constant} . \tag{47}$$

E. The Legendre Polynomial Expansion of $\Phi(E,x,\mu)$

We now expand $\varphi_s(E,\mu)$, $\Psi_{2;s}(E,\mu)$ and $\delta(\hat{v} \cdot \hat{v} - g(E',E))$ in Legendre polynomials; specifically,

$$\varphi_s(E,\mu) = \mu \sum_{m=0}^{\infty} \frac{2m+1}{2} \varphi_{s,m}(E) P_m(\mu) , \tag{48}$$

$$\Psi_{2;s}(E,\mu) = \mu \sum_{m=0}^{\infty} \frac{2m+1}{2} \Psi_{2;s,m}(E) P_m(\mu) \tag{49}$$

and

$$\begin{aligned} \delta(\hat{v} \cdot \hat{v}' - g) = & \sum_{m=0}^{\infty} \frac{2m+1}{2} P_m(g) \{ P_m(\mu) P_m(\mu') \\ & + 2 \sum_{r=0}^{m} \frac{(m-r)!}{(m+r)!} P_m{}^r(\mu) P_m{}^r(\mu') \cos(\varphi - \varphi') \} . \end{aligned} \tag{50}$$

By substituting these expansions into Eq. (44) and performing angular integrations, we obtain a coupled set of integral equations for the $\varphi_{n,\ell}$;

$$\begin{aligned} & - 2n [\frac{\ell}{2\ell+1} \varphi_{n-1,\ell-1}(E) + \frac{2+1}{2\ell+1} \varphi_{m-1,\ell+1}(E)] + \xi(E) N \sigma^T(E) \varphi_{n,\ell}(E) \\ & = V_{n,\ell}(E) + W_{n,\ell}(E) + \int_E^{\beta E} dE' \mathcal{F}(E',E) P_\ell(g(E',E)) Q_{n,n}(E',E) \varphi_{n,\ell}(E') , \end{aligned} \tag{51}$$

where

$$V_{n,\ell}(E) = \sum_{s=0}^{n} \int_{E}^{\beta E} dE' \mathcal{F}(E',E) P_{\ell}(g(E',E)) \times Q_{n,s}(E',E) \Psi_{2;s,\ell}(E') \tag{52}$$

$$W_{n,\ell}(E) = \sum_{s=0}^{n-1} \int_{E}^{\beta E} dE' \mathcal{F}(E',E) P_{\ell}(g(E',E)) \times Q_{n,s}(E',E) \varphi_{g,\ell}(E') . \tag{53}$$

An explicit expression for $\Psi_{2;s,\ell}(E)$ is derived in Appendix C. Although Eq. (51) describes a set of coupled equations, the coupling is such that the $\varphi_{n,\ell}(E)$ may be obtained, order by order, in a natural sequence. The equations for the functions $\varphi_{o,\ell}(E)$ are uncoupled,

$$\xi(E) N \sigma^{T}(E) \varphi_{o,\ell}(E) = V_{o,\ell}(E) + \int_{E}^{\beta E} dE' \mathcal{F}(E',E) Q_{o,o}(E',E) \varphi_{o,\ell}(E') , \tag{54}$$

and so these functions may be obtained directly, say for a set $\ell = 0, 1, \ldots, \overline{\ell}$. The equations for the $\varphi_{1,\ell}(E)$ depend on $\varphi_{o,m}$, $m = 0, 1, \ldots, \ell + 1$, and so $\varphi_{1,\ell}$ may now be found for the set of ℓ values $\ell = 0, 1, \ldots, \overline{\ell} - 1$. This process is then continued until $\varphi_{\overline{\ell},o}$ is determined. If at that point we see that more terms are needed, we can solve successively for $\varphi_{o,\overline{\ell}+1}$, $\varphi_{1,\overline{\ell}}$, ..., $\varphi_{\overline{\ell}+1,o}$ without modifying the solutions for the terms obtained previously.

Equation (51) is modified, of course, when the inelastic loss term in the Boltzmann equation is taken into account. The form of the equation remains unchanged however and the procedure for its solution is unaffected. Details of the changes introduced by including the contributions of the inelastic losses are given in Appendix A.

The matrix inversion method for solving the integral equations for the $\varphi_{n,\ell}$ is described in detail in Appendix D.

F. Calculation for 200 keV Antimony Atoms Incident on Germanium

In our calculation we used the Winterbon analytical fit[7] to the LNS[10] elastic cross section, with however two modifications. The Winterbon fit to the elastic cross section diverges at small energy transfers as $t^{-4/3}$; we have therefore introduced a low-energy transfer cut off T, at 14.5 eV, a reasonable estimate for the energy needed to displace a germanium atom. With this cut off however, the total cross section goes to zero precipitously at T . As is pointed out in Appendix D, this introduces difficulties with the numerical solution for $\varphi_{n,\ell}$. We therefore introduced one further modification in the cross section below 100 eV which allows the total cross section to go to zero smoothly with energy. Both modifications are described in detail in Appendix E. We use the LSS[6] evaluation of the inelastic stopping power, but again with a modification introduced for numerical convenience at energies below 100 eV. These alterations, because they are made at energies so low compared to the incident energy, do not alter quantities of physical interest such as range and deposited energy distribution to any significant extent.

As stated earlier we have found it expedient to neglect the effect of inelastic energy loss on Ψ_0, Ψ_1, and Ψ_2. The depth distribution of electronic energy loss near the surface will of course be adversely affected, but Ψ itself, and therefore elastic losses, is hardly affected at all. As an illustration, in Fig. 1 we plot Ψ_1 integrated over energy (the energy dependence is set by the δ-function) as a function of angle for the case where inelastic losses are included and also where they are neglected. Albeit it is a log plot, the results are indistinguishable.

The functions $\overline{x}(E)$ and $\xi(E)$ were determined by a quasi-self-consistent method. A physically reasonable form was initially chosen, and Eq. (51) (modified according to Eq. (A12)) was solved for the $\varphi_{n,\ell}(E)$. Moments of the range distribution of beam particles having energy E were then calculated (see Appendix F) and a new analytical fit for $\overline{x}(E)$ and $\xi(E)$ obtained. No further iteration was found necessary. Figure 2 depicts the energy dependence of $\overline{x}$ and ξ found in this way.

Expressions for the distribution of stopped ions and for the distribution of energy deposited in elastic collisions are derived in Appendix F. It is shown there that these distributions depend only on $\varphi_{n,o}$ and $\Psi_{2;n,o}$. The range and deposited energy distributions shown in Figs. 3 and 4 include contributions for values of n up through 7. At that point the Hermite expansion has not yet quite converged, but the resultant distributions should be good to about 10%.

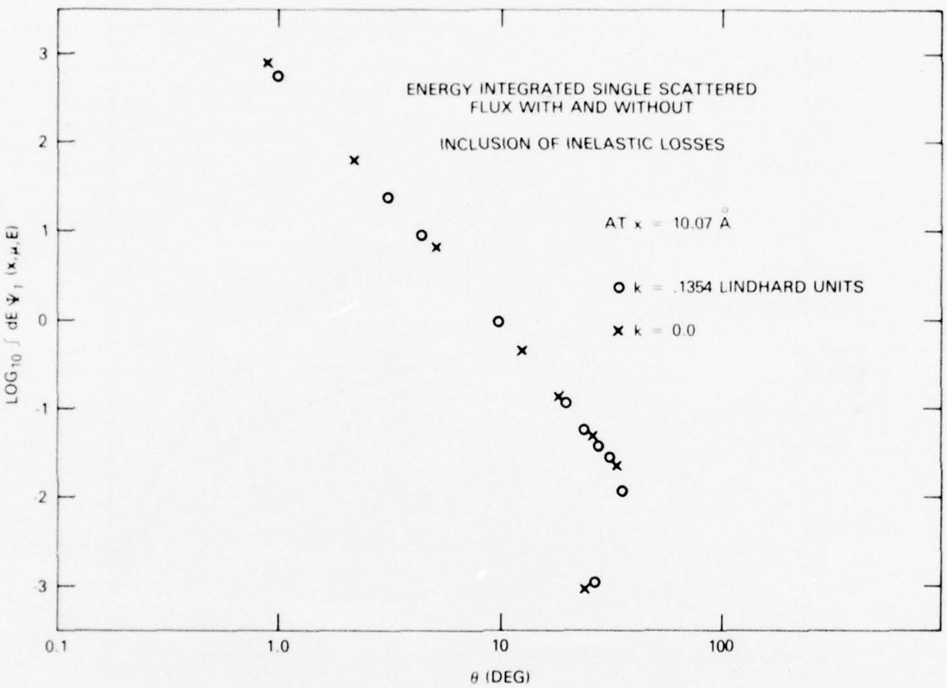

Fig. 1 — The flux of once scattered particles integrated over energy with and without the inclusion of inelastic losses. An inelastic loss proportional to velocity is used, with a value of k of .1354 Lindhard units.

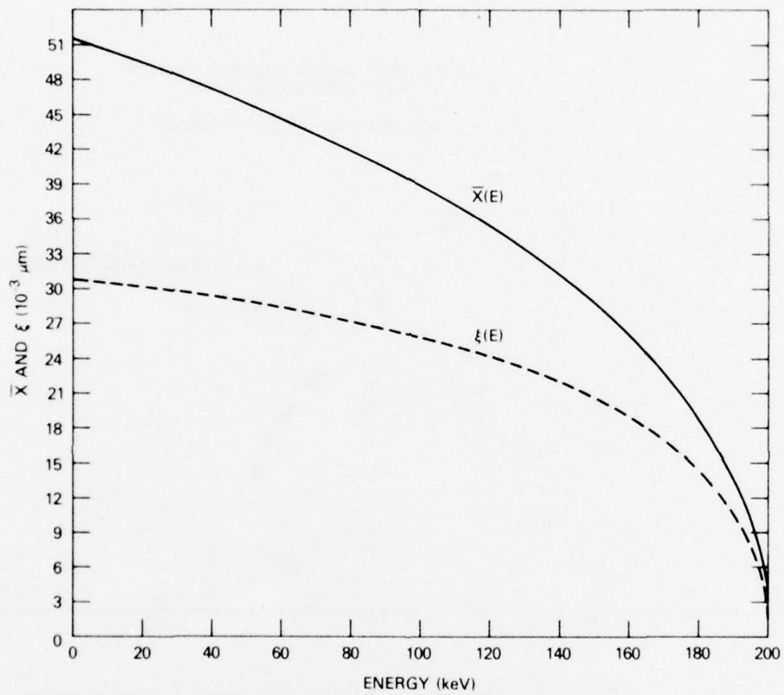

Fig. 2 — The energy dependence of the parameters $\overline{x}$ and ξ

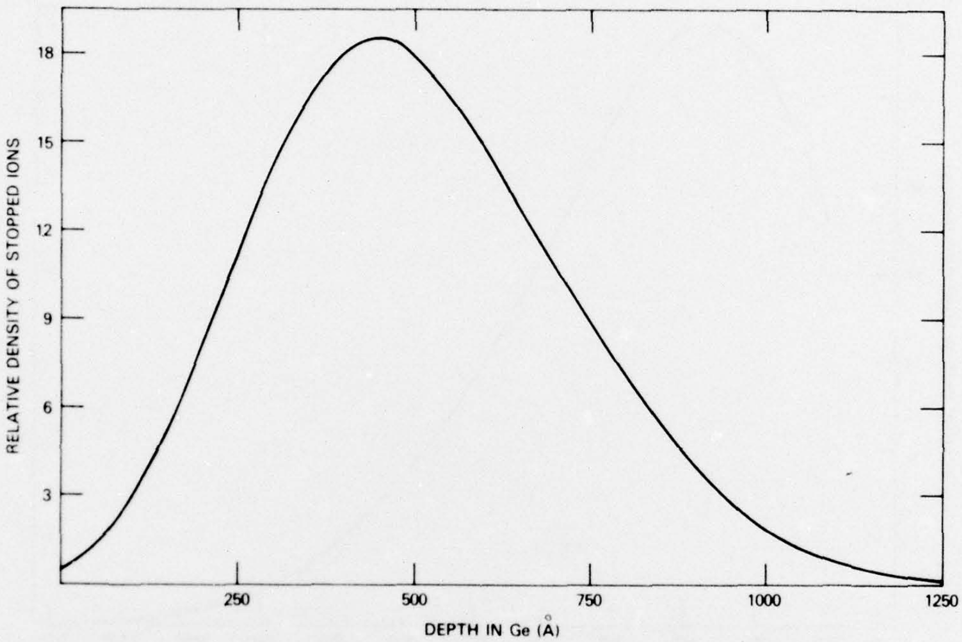

Fig. 3 — The depth distribution of stopped beam ions for the case of a 200 keV monoenergetic beam of antimony ions normally incident on germanium

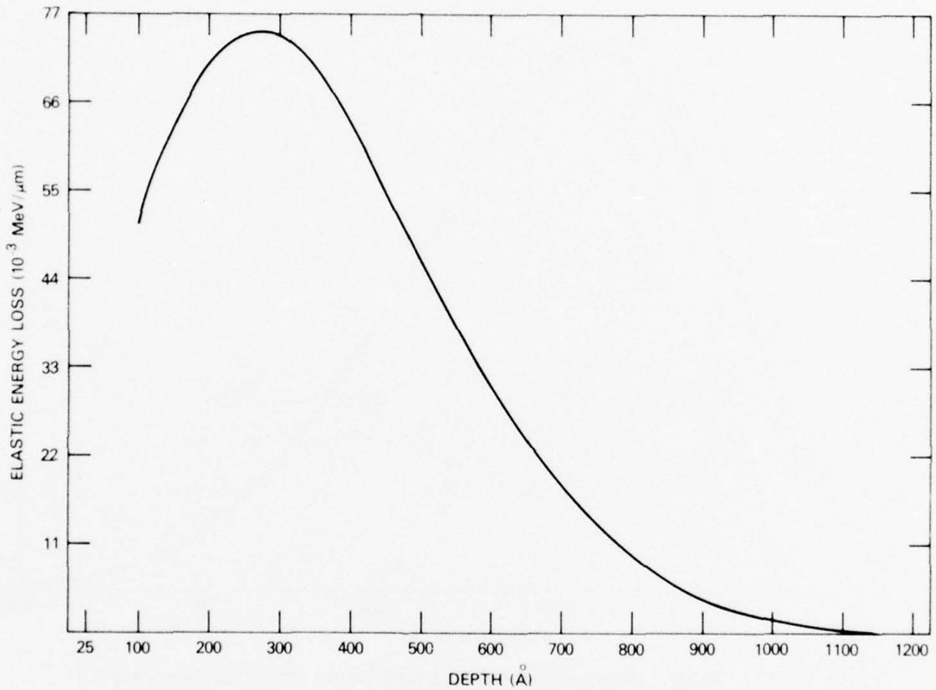

Fig. 4 — The depth distribution of energy loss from the incident antimony beam in elastic collisions with germanium atoms

Appendix A. Inclusion of Inelastic Losses

As indicated in the text, inelastic losses (in the continuous slowing down approximation) are taken into account by including a term

$$I(E,x,\mu) = -\frac{\partial}{\partial E}(S(E)\Phi(E,x,\mu)) \tag{A1}$$

on the left hand side of Eq. (23), where S(E) is the inelastic stopping power. In order to obtain the alterations made by this term to Eq. (51), we expand Φ in Hermite and Legendre polynomials. First we make the Legendre expansion shown in Eq. (48),

$$\Phi(E,x,\mu) = \mu \sum_{\ell=0} \frac{2\ell+1}{2} \varphi_\ell(E,x) P_\ell(\mu) \; . \tag{A2}$$

We divide by $2/(2\ell + 1)$ to find the contribution of the ℓth harmonic to the transport equation is

$$I_\ell(E,x) = -\frac{\partial}{\partial E}(S(E)\varphi_\ell(E,x)) \; . \tag{A3}$$

We now introduce the Hermite expansion of φ_ℓ,

$$\varphi_\ell(E,x) = \sum_{m=0} h_m^{-1} \varphi_{m,\ell}(E) e^{-y^2} H_m(y) , \tag{A4}$$

where

$$y = (x - \overline{x})/\xi \; . \tag{A5}$$

Now the Hermite polynomials satisfy the relation

$$\frac{d}{dy}(H_m(y) e^{-y^2}) = -H_{m+1}(y) e^{-y^2} , \tag{A6}$$

and therefore

$$I_\ell(E,x) = -S'(E)\sum_{m=0} h_m^{-1}\varphi_{m,\ell}(E)\,e^{-y^2}H_m(y)$$

$$- S(E)\sum_{m=0} h_m^{-1}\varphi'_{m,\ell}(E)\,e^{-y^2}H_m(y) + \sum_{m=0} h_m^{-1}\varphi_{m,\ell}(E)\,e^{-y^2}H_{m+1}(y)\times$$

$$\times\left[-\frac{\bar{x}}{\xi} - \frac{\xi'}{\xi}\,\frac{(x-\bar{x})}{\xi}\right]. \tag{A7}$$

Using the recurrence relation

$$2yH_m(y) = H_{m+1}(y) + 2m\,H_{m-1}(y)\ , \tag{A8}$$

we obtain

$$I_\ell(E,x) = e^{-y^2}\sum_{m=0}\{[-S'(E)\varphi_{m,\ell}(E) - S(E)\varphi'_{m,\ell}(E)$$

$$-\frac{(m+1)\xi'S(E)}{\xi}\varphi_{m,\ell}(E)]\,H_m(y)$$

$$-\frac{\bar{x}'S(E)}{\xi}\varphi_{m,\ell}(E)H_{m+1}(y)$$

$$-\frac{\xi'S(E)}{2\xi}\varphi_{m,\ell}(E)H_{m+2}(y)\}\ . \tag{A9}$$

Operating on I_ℓ by $\xi(E)\int_{-\infty}^{\infty} dy\ H_n(y)$, we find

$$I_{n,\ell}(E) = -\xi\{[S'(E) + (n+1)\frac{\xi'}{\xi}]\varphi_{n,\ell}(E) + S(E)\varphi'_{n,\ell}(E)$$

$$+ \frac{\bar{x}'}{\xi}\frac{h_n}{h_{n-1}}\varphi_{n-1,\ell}(E) + \frac{\xi'}{2\xi}\frac{h_n}{h_{n-2}}\varphi_{n-2,\ell}(E)\}. \tag{A10}$$

Now

$$h_n = \sqrt{\pi}\,2^n n!\,, \tag{A11}$$

thus

$$I_{n,\ell}(E) = -\xi\{[S'(E) + (n+1)\frac{\xi' S(E)}{\xi}]\varphi_{n,\ell}(E)$$

$$+ S(E)\varphi'_{n,\ell}(E) + 2n\frac{\bar{x}' S(E)}{\xi}\varphi_{n-1,\ell}(E) \tag{A12}$$

$$+ 2n(n-1)\frac{\xi' S(E)}{\xi}\varphi_{n-2,\ell}(E)\}.$$

Appendix B. Evaluation of $Q_{n,s}(E',E)$

In this appendix we evaluate the function

$$Q_{n,s}(E',E) = h_s^{-1} \int_{-\infty}^{\infty} dx\, H_n(y) H_s(y') e^{-y'^2} \tag{B1}$$

which appears in Eqs. (44) and (51) and where

$$\begin{aligned} h_s &= \sqrt{\pi}\, 2^s s! \\ y &= (x - \bar{x})/\xi \\ y' &= (x - \bar{x}')/\xi', \end{aligned} \tag{B2}$$

and where the H_n are Hermite polynomials of order n.

We first rewrite Eq. (B1)

$$Q_{n,s}(E',E) = (\xi'/h_s) \int_{-\infty}^{\infty} dy' e^{-y'^2} H_s(y') H_n\left(\frac{\xi'}{\xi} y' + \frac{(\bar{x}' - \bar{x})}{\xi}\right). \tag{B3}$$

We remark that

$$Q_{n,s}(E',E) = 0,\ s > n\ , \tag{B4}$$

and use the fact that

$$2^{\frac{n}{2}} H_n(x + y) = \sum_{m=0}^{n} \binom{n}{m} H_m(\sqrt{2}\,x) H_{n-m}(\sqrt{2}\,y) \tag{B5}$$

to obtain

$$Q_{n,s}(E',E) = 2^{-\frac{n}{2}} \xi'/h_s \sum_{m=s}^{n} \binom{n}{m} H_{n-m}\left(\sqrt{2}\ \frac{\overline{x}' - \overline{x}}{\xi}\right) \times$$

$$\times \int_{-\infty}^{\infty} dy' \, e^{-y'^2} H_s(y') H_m\left(\sqrt{2}\ y' \ \frac{\xi'}{\xi}\right) . \tag{B6}$$

The integral can be done explicitly,[10] and with a change of summation index $m = s + 2r$, we obtain

$$Q_{n,s}(E',E) = \xi'(2^{n/2} s!)^{-1} \left(\sqrt{2}\ \frac{\xi'}{\xi}\right)^s \times$$

$$\times \sum_{r=0}^{\left[\frac{n-s}{2}\right]} \frac{n!}{r!\,(n-s-2r)!} \left[2\left(\frac{\xi'}{\xi}\right)^2 - 1\right]^r \times$$

$$\times H_{n-s-2r}\left(\sqrt{2}\ \frac{\overline{x}' - \overline{x}}{\xi}\right) , \tag{B7}$$

where the upper limit of the summation $[(n-s)/2]$ denotes the greatest integer less than or equal to $(n-s)/2$.

Appendix C. Evaluation of $\Psi_{2;n,\ell}(E)$

By definition $\Psi_{2;n,\ell}(E)$ is related to $\Psi_2(E,x,\mu)$ by the expression

$$\Psi_{2;n,\ell}(E) = \int_{-1}^{1} d\mu \, \frac{1}{\mu} \, P_\ell(\mu) \xi^{-1} \int_{-\infty}^{\infty} dx \, H_n\left(\frac{x - \bar{x}}{\xi}\right) \Psi_2(E,x,\mu) \, . \qquad (C1)$$

To obtain a numerically useful expression for $\Psi_{2;n,\ell}$ however, the best method is not the most direct one where Ψ_2 is taken from Eq. (38). Rather it is better to start with the defining equation for $\Psi_2(E,x,\mu)$

$$\mu \frac{\partial}{\partial x} \Psi_2 + \sigma^T(E)\Psi_2 = \frac{\mu}{2\pi} \int_E^{\beta E} dE' \mathcal{F}(E',E)\psi_1(E',x) \times$$

$$\times \int d\hat{v}' \delta(\hat{v} \cdot \hat{v}' - g_1) \, \mu'^{-1} \delta(\mu' - g_2), \qquad (C2)$$

where
$$g_1 = g(E',E) \text{ and } g_2 = g(E_B,E') \qquad (C3)$$

and $g(E_1,E_2)$ is the cosine of the laboratory scattering angle for a beam atom entering with energy E_1 and leaving with energy E_2. After we expand the δ-function

$$\delta(\hat{v} \cdot \hat{v}' - g_1) = \sum_{\ell=0} \frac{2\ell+1}{2} P_\ell(g_1)[P_\ell(\mu)P_\ell(\mu')$$

$$+ \sum_{m=1}^{\ell} \frac{(\ell - m)!}{(\ell + m)!} P_\ell^m(\mu) P_\ell^m(\mu') \cos m(\varphi - \varphi')] \qquad (C4)$$

the integrations over φ' and μ' can be done immediately to yield for the RHS of Eq. (C2)

$$\text{RHS} = \int_E^{\beta E} dE' \; \frac{\mathcal{F}(E',E)\psi_1(E',x)}{g(E_B,E')} \sum_\ell \frac{2\ell+1}{2} P_\ell(g_1) P_\ell(g_2)\, \mu\, P_\ell(\mu). \tag{C5}$$

Now expand Ψ_2,

$$\Psi_2(E,x,\mu) = \mu \sum_\ell \frac{2\ell+1}{2} \Psi_{2;\ell}(E,x) P_\ell(\mu) . \tag{C6}$$

If we note that

$$\begin{aligned}\mu \frac{\partial}{\partial x} \Psi_2 &= \sum_{\ell=0} \frac{2\ell+1}{2} \frac{\partial}{\partial x} \Psi_{2;\ell}(E,x)\, \mu^2 P_\ell(\mu) \\ &= \sum_{\ell=0} \left[\frac{\ell}{2} \frac{\partial}{\partial x} \Psi_{2;\ell-1} + \frac{\ell+1}{2} \frac{\partial}{\partial x} \Psi_{2;\ell+1} \right] \mu P_\ell(\mu),\end{aligned} \tag{C7}$$

we obtain

$$\begin{aligned}&\frac{\ell}{2\ell+1} \frac{\partial}{\partial x} \Psi_{2;\ell-1}(E,x) + \frac{\ell+1}{2\ell+1} \frac{\partial}{\partial x} \Psi_{2;\ell+1}(E,x) + \sigma^T(E)\Psi_{2;\ell}(E,x) \\ &= \int_E^{\beta E} dE' \; \frac{\mathcal{F}(E',E)\psi_1(E',x)}{g_2} P_\ell(g_1) P_\ell(g_2) .\end{aligned} \tag{C8}$$

We now expand $\Psi_{2,\ell}(E,x)$ in Hermite polynomials. We let

$$y = (x - \bar{x})/\xi , \tag{C9}$$

and write

$$\Psi_{2;\ell}(E,x) = \sum_{n=0} h_n^{-1} \Psi_{2;n,\ell}(E) H_n(y) e^{-y^2} , \tag{C10}$$

where

$$h_n = \sqrt{\pi}\, 2^n n! \; . \tag{C11}$$

We substitute this sum for $\Psi_{2;\ell}$ in Eq. (C8), note that

$$\frac{\partial}{\partial x}\left(e^{-y^2} H_n(y)\right) = -\xi^{-1} e^{-y^2} H_{n+1}(y) \tag{C12}$$

and use the orthonormality property of the Hermite polynomials,

$$\int_{-\infty}^{\infty} dy\, e^{-y^2} H_s(y) H_n(y) = h_s \delta_{sn} \tag{C13}$$

to obtain

$$(-2s)\left[\frac{\ell}{2\ell+1}\Psi_{2;s-1,\ell-1} + \frac{\ell+1}{2\ell+1}\Psi_{2;s-1,\ell+1}\right]$$

$$+ \xi\, \sigma^T(E) \Psi_{2;s,\ell} \tag{C14}$$

$$= \int_E^{\beta E} dE' \, \frac{\mathcal{F}(E',E) P_\ell(g_1) P_\ell(g_2)}{g_2} \int_{-\infty}^{\infty} dx\, \psi_1(E',x) H_s(y) \; .$$

Taking ψ_1 from Eqs. (26) and (27) and noting that

$$2^{\frac{s}{2}} H_s\left(\frac{x}{\xi} - \frac{\bar{x}}{\xi}\right) = \sum_{k=0}^{s} \binom{s}{k} H_k\left(\sqrt{2}\,\frac{x}{\xi}\right) H_{s-k}\left(-\sqrt{2}\,\frac{\bar{x}}{\xi}\right) \tag{C15}$$

and

$$\int_0^{\infty} d\eta\, H_k(\sqrt{2}\,\eta)\, e^{-\alpha\eta} = \frac{k!}{\alpha} \sum_{\nu=0}^{[\frac{k}{2}]} \frac{(-1)^\nu}{\nu!} \left(\frac{2^{\frac{3}{2}}}{\alpha}\right)^{k-2\nu} , \tag{C16}$$

where the symbol $[k/2]$ denotes the largest integer contained in $k/2$, we find that

$$\int_{-\infty}^{\infty} dx\,\psi_1(E',x)H_s(y) = 2^{-\frac{s}{2}}\,\frac{\mathcal{F}(E_B,E')}{\ell_B\ell(E')}\sum_{k=0}^{s}\frac{s!}{(s-k)!}H_{s-k}\left(-\sqrt{2}\,\frac{\bar{x}}{\xi}\right)\times$$

$$\times\sum_{\nu=0}^{[\frac{k}{2}]}\frac{(-1)^{\nu}}{\nu!}\left(\frac{2^{\frac{3}{2}}}{\ell_B\xi}\right)^{k-2\nu}\sum_{\mu=0}^{k-2\nu}\left(\frac{\ell_B}{\ell(E')}\right)^{\mu}, \tag{C17}$$

where

$$\ell_B = \sigma^T(E_B) \text{ and } \ell(E') = \sigma^T(E')/g_2 . \tag{C18}$$

The final result then is

$$(-2s)\left[\frac{\ell}{2\ell+1}\Psi_{2;s-1,\ell-1}(E) + \frac{\ell+1}{2\ell+1}\Psi_{2;s-1,\ell+1}(E)\right] + \xi\sigma^T(E)\Psi_{2;s,\ell}(E)$$

$$= \frac{2^{-\frac{s}{2}}}{\ell_B}\sum_{k=0}^{s}\frac{s!}{(s-k)!}H_{s-k}\left(-\sqrt{2}\,\frac{\bar{x}}{\xi}\right)\sum_{\nu=0}^{[\frac{k}{2}]}\frac{(-1)^{\nu}}{\nu!}\left(\frac{2^{\frac{3}{2}}}{\ell_B\xi}\right)^{k-2\nu}\times \tag{C19}$$

$$\times\sum_{\mu=0}^{k-2\nu}\int_E^{\beta E} dE'\,\frac{\mathcal{F}(E_B,E')\mathcal{F}(E',E)}{\sigma^T(E')}P_\ell(g_1)P_\ell(g_2)\left(\frac{\ell_B}{\ell(E')}\right)^{\mu} \equiv U_{s,\ell}(E) .$$

We have therefore

$$\Psi_{2;0,\ell}(E) = U_{0,\ell}(E)/\xi\sigma^T(E)$$

$$= \frac{1}{\xi\sigma^T(E)\ell_B}\int_E^{\beta E} dE'\,\frac{\mathcal{F}(E_B,E')\mathcal{F}(E',E)}{\sigma^T(E')}P_\ell(g(E_B,E'))P_\ell(g(E',E)) \tag{C20}$$

and

$$\xi\sigma^T(E)\Psi_{2;n,\ell}(E) = 2n\left[\frac{\ell}{2\ell+1}\Psi_{2;n-1,\ell-1}(E) + \frac{\ell+1}{2\ell+1}\Psi_{2;n-1,\ell+1}(E)\right] + U_{n,\ell} . \tag{C21}$$

Appendix D. Numerical Solution of the Integral Equation

In this appendix we describe how the integral equation for $\varphi_{o,o}(E)$ is solved. This will serve as an illustration of how the equations for all the $\varphi_{n,\ell}(E)$ are solved. For the purposes of this section we will neglect inelastic losses (but will indicate at the end how they are treated) and will assume the cross section is given by the Winterbon, Sigmund and Sanders[7] analytical fit to the Lindhard, Nielsen and Scharff[10] cross section. Since the LNS cross section becomes singular as the energy transfer goes to zero, we introduce a cutoff T to represent a minimum energy transfer allowed in an elastic collision. The method described below works equally well, moreover, with other cross sections.

With the use of the LNS cross section, the function $\varphi_{o,o}(E)$ satisfies the equation

$$\begin{aligned} \xi\sigma^T(E)\varphi_{o,o}(E) &= V_{o,o}(E) \\ &+ \int_{E+T}^{\beta E} dE'\, U(E_B - 3T - E')\xi'\mathcal{F}(E',E')\varphi_{o,o}(E') , \end{aligned} \tag{D1}$$

where all of the terms appearing here have been defined in the body of this report. If we define

$$m(E) = \min[\beta E, E_B - 3T] , \tag{D2}$$

then we have

$$\begin{aligned} \xi\sigma^T(E)\varphi_{o,o}(E) &= V_{o,o}(E) \\ &+ \int_{E+T}^{m(E)} dE'\xi'\mathcal{F}(E',E)\varphi_{o,o}(E') . \end{aligned} \tag{D3}$$

Briefly, given an appropriate energy mesh $\{E_j\}$, our aim is to express Eq. (D3) as a set of linear equations in the set $\{\varphi_{o,o}(E_j)\}$, which we will then solve by straightforward matrix inversion.

Consider the integral in Eq. (D3). We carry out the integration using Gauss-Legendre quadrature. Thus if $\{z_j\}$ and $\{w_i\}$ are the sets of Gauss-Legendre ordinates and weights, respectively, for n-point integration, then the integral in Eq. (D3) may be expressed

$$\int_{E_j+T}^{m(E_j)} dE' \xi(E')\mathcal{F}(E',E_j)\varphi_{o,o}(E') = R(E_j)\sum_{i=1}^{n} w_i \xi(\mathcal{E}_{ji})\mathcal{F}(\mathcal{E}_{ji},E_j)\varphi_{o,o}(\mathcal{E}_{ji}), \tag{D4}$$

where

$$\mathcal{E}_{ji} = B(E_j) + R(E_j)z_i \tag{D5}$$

and

$$R(E) = \tfrac{1}{2}[m(E) - (E+T)], \; B(E) = \tfrac{1}{2}(m(E) + E + T) . \tag{D6}$$

This method fails when singularities (or near singularities) occur in the integrand; when such is the case, the singularities should be removed before integrating. For example, the WSS[7] representation of the LNS[10] cross section is proportional to $(E' - E)^{-4/3}$, that is,

$$\mathcal{F}(E',E) = G(E',E)/(E' - E)^{4/3} , \tag{D7}$$

where $G(E',E)$ is well behaved. In this case the singularity is removed by introducing the change of variable $y = (E' - E)^{-1/3}$, so that

$$\int_{E+T}^{m(E)} dE'\xi(E)\mathcal{F}(E',E)\varphi_{o,o}(E')$$

$$= 3\int_{[m(E)-E]^{-1/3}}^{T^{-1/3}} dy\,\xi(E+y^{-3})\mathcal{F}(E+y^{-3},E)\varphi_{o,o}(E+y^{-3}) . \tag{D8}$$

The new integral contains no singularities and can be evaluated as described above. Another, not so obvious, singularity is associated with the LNS cross section and with the cutoff T; as E approaches T/γ, where

$$\gamma = \frac{4M}{(1+M)^2} \tag{D9}$$

the total cross section $\sigma^T(E)$ rapidly goes to zero. The left side of Eq. (D3) remains finite, however. This means that $\varphi_{o,o}(E)$ is increasing just as fast as $\sigma^T(E)$ is decreasing. We have handled this situation by modifying the LNS cross section at energies less than 100 eV so that this sharp cutoff of $\sigma^T(E)$ does not occur. The modification is described in Appendix E.

Let us assume that all singularities have already been removed in Eq. (D3). Then for each mesh point E_j we have

$$\xi(E_j)\sigma^T(E_j)\varphi_{o,o}(E_j) = V_{o,o}(E_j)$$
$$+ R(E_j)\sum_{i=1}^{n} w_i\xi(\mathcal{E}_{ji})\mathcal{F}(\mathcal{E}_{ji},E_j)\varphi_{o,o}(\mathcal{E}_{ji}) . \tag{D10}$$

Generally, the argument of $\varphi_{o,o}$ on the right side will lie among the

mesh points $\{E_j\}$. We use cubic spline interpolation to express

$$\varphi_{o,o}(\mathcal{E}_{ji}) = \sum_k C_k^{ij} \varphi_{o,o}(E_k) , \tag{D11}$$

where the coefficients C_k^{ij} are determined by the cubic spline equations and found without having to know the values $\varphi_{o,o}(E_k)$. Equation (D10), which now describes a set of linear equations in $\{\varphi_{o,o}(E_k)\}$, therefore has the form

$$\sum_k A_{jk} \varphi_{o,o}(E_k) = V_{o,o}(E_j) , \tag{D12}$$

where

$$\begin{aligned} A_{jk} &= \xi(E_j)\sigma^T(E_j)\delta_{jk} \\ &\quad - R(E_j) \sum_{i=1}^{n} w_i \xi(\mathcal{E}_{ji}) \mathcal{F}(\mathcal{E}_{ji}, E_j) C_k^{ij} . \end{aligned} \tag{D13}$$

The desired solution is then

$$\varphi_{o,o}(E_k) = \sum_j A_{kj}^{-1} V_{o,o}(E_j) . \tag{D14}$$

As a test of the accuracy of the method, we considered the equation

$$D(E) = V(E) + \int_{E+T}^{m(E)} dE' K(E',E) D(E') , \tag{D15}$$

with

$$K(E',E) = [1 + (E'-E)^{4/3}]/(E'-E)^{4/3} . \tag{D16}$$

The function V(E) is a rather complex function of E and T, such that the solution of Eq. (D17) is

$$D(E) = (E_B - 3T - E)^2 . \tag{D17}$$

By employing the method described above, a mesh of 42 energy points, and 32 Gauss-Legendre points, we reproduced the exact solution at all the mesh points to an accuracy of better than 10^{-6} per cent.

In Appendix A, we have shown that inelastic losses are taken into account by adding a term $I_{n,\ell}(E_j)$ to the left hand side of Eq. (D10), where

$$\begin{aligned} I_{n,\ell}(E) = -\xi(E)\{[S'(E) + (n+1)\frac{\xi'}{\xi} S(E)]\varphi_{n,\ell}(E) + S(E)\varphi'_{n,\ell}(E) \\ + 2n\frac{\bar{x}'}{\xi} S(E)\varphi_{n-1,\ell}(E) + 2n(n-1)\frac{\xi'}{\xi} S(E)\varphi_{n-2,\ell}(E)]\} , \end{aligned} \tag{D18}$$

where S(E) is the inelastic stopping power and the "prime" denotes the derivative with respect to energy. From the cubic spline equations, we obtain $\varphi'_{n,\ell}(E_j)$

$$\varphi'_{n,\ell}(E_j) = \sum_i D_{ji}\varphi_{n,\ell}(E_i) . \tag{D19}$$

The resulting equations can then be solved as indicated above by straightforward matrix inversion.

Appendix E. Modification of LNS Cross Section and LSS Inelastic Stopping Power at Low Energy

1. Cross Section Modification

The unmodified LNS elastic scattering cross section is given by

$$\mathcal{F}^{(u)}_{LNS}(E',E) = \frac{N\pi a^2}{2\gamma E_L^2} E' t^{-3/2} f(t^{1/2}) U(\beta E - E') , \qquad (E1)$$

where a is the Lindhard screening length, E_L is the Lindhard energy,

$$t = \frac{E'T}{\gamma E_L^2} , \quad T = E' - E , \qquad (E2)$$

$f(t^{1/2})$ is given, in the Winterbon approximation, by

$$f(t^{1/2}) = 1.309\, t^{1/6} [1 + (2.618\, t^{2/3})^{2/3}]^{-3/2} , \qquad (E3)$$

the step function $U(\beta E - E')$ merely expresses the kinematical elastic scattering condition that the initial energy of the scattered particle, E, is greater than the minimum possible value of the outgoing energy. All other symbols are defined in the body of the paper. The cutoff at low energy transfers is introduced by multiplying Eq. (E1) by another step function

$$\mathcal{F}_{LNS}(E',E) = \frac{N\pi a^2}{2\gamma E_L^2} E' t^{-3/2} f(t^{1/2}) U(\beta E - E') U(E' - E - T_c) , \qquad (E4)$$

where T_c is the cutoff energy transfer. For expediency in the numerical solution of the integral equations, we also wanted the total cross section to vanish smoothly at low energies and so we introduced one other modification for energies less than an energy $\bar{E}$ (which we took

to be 100 eV),

$$\mathcal{F}(E',E) = \begin{cases} \mathcal{F}_{LNS}(E',E) & , E' > \overline{E} \\ \mathcal{F}_{LNS}(E',E) \dfrac{U\left(E' - \dfrac{E\overline{E}}{\overline{E} - T_c}\right)}{U(E' - E - T_c)} & , E' < \overline{E} . \end{cases} \tag{E5}$$

In Fig. 5 we show the energy dependence at low energies of both the modified and unmodified LNS total cross sections (both including the low energy transfer cutoff at $T_c = 14.5$ eV).

2. Inelastic Stopping Power

The LSS elastic stopping power is proportional to the particle velocity

$$S(E) = K E^{1/2} , \tag{E6}$$

where, for the case of antimony on germanium, we take $K = 1.32$ MeV$^{1/2}$/μm. For numerical convenience we have added an additional term at low energy

$$S_{mod}(E) = 0.2 \left(\frac{\overline{E} + E}{\overline{E}}\right)^3 \left(\frac{\overline{E} - E}{\overline{E}}\right)^2 \text{MeV}/\mu\text{m} , \tag{E7}$$

so that

$$S(E) = \begin{cases} K E^{1/2} & , E > \overline{E} \\ K E^{1/2} + S_{mod}(E) & , E \leq \overline{E} , \end{cases} \tag{E8}$$

where again we have taken $\overline{E} = 100$ eV.

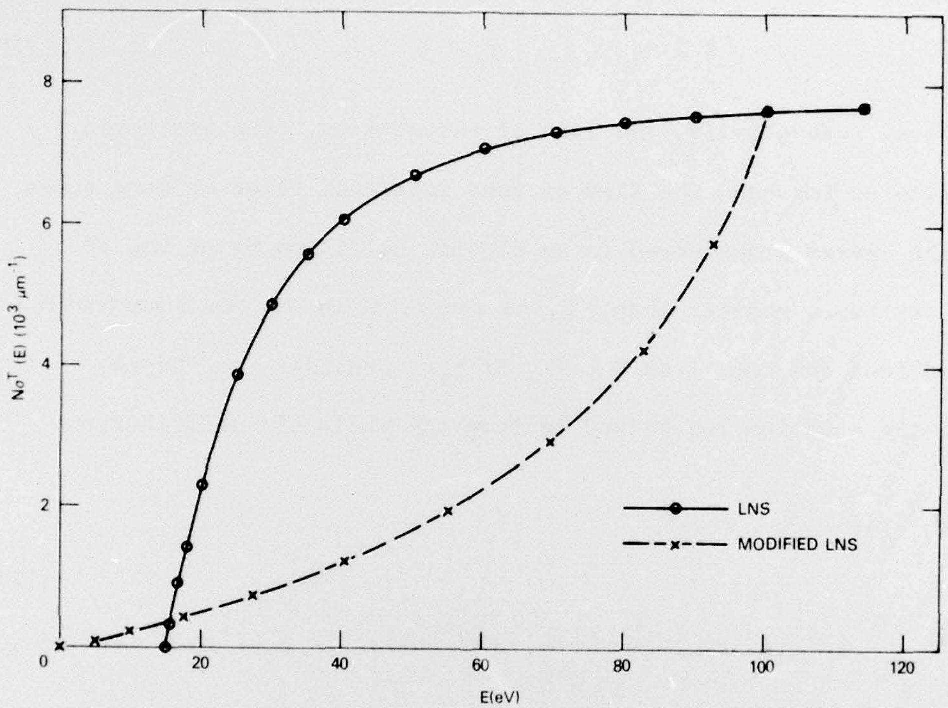

Fig. 5 — The dependence at low energies of both the LNS total cross section and its modification used in the present calculation

Appendix F. Range and Deposited Energy Distributions and Their Moments

1. Distribution of Stopped Beam Ions

As stated in the body of the text, we have written Ψ as the sum of four terms,

$$\Psi = \Psi_0 + \Psi_1 + \Psi_2 + \Phi , \tag{F1}$$

representing, respectively, the flux of unscattered, once scattered, twice scattered ions and the flux of ions scattered three or more times. Because the energy transferred in an elastic collision by an ion of energy E can be no greater than γE, no contribution to the distribution of stopped ions can come from Ψ_0, Ψ_1, or Ψ_2. Consider, therefore, Eq. (23), the equation for φ (and include the inelastic contribution)

$$\mu \frac{\partial \Phi}{\partial x} + N\sigma^T(E)\Phi - \frac{\partial}{\partial E}(S(E)\Phi)$$

$$= \frac{\mu}{2\pi}\int_E^{\beta E} dE'\mathcal{F}(E',E)\int d\hat{v}'\delta(\hat{v}\cdot\hat{v}' - g(E',E))\mu'^{-1}[\Psi_2(E',x,\mu' + \Phi(E',x,\mu')] . \tag{F2}$$

The x component of the current of particles scattered three or more times

$$j(x) = \int_{-1}^{1} d\mu \int_0^{E_B - 3T} dE\,\Phi(E,x,\mu) \tag{F3}$$

must obey a particle conservation rule

$$\frac{dj(x)}{dx} + \frac{d\sigma(x)}{dx} + \frac{d\tau(x)}{dx} = 0 , \tag{F4}$$

where $d\sigma(x)/dx$ is the distribution of stopped beam ions and $d\tau(x)/dx$

is the distribution of twice scattered particles which are elastically scattered a third time in the interval between x and x + dx. If we operate on Eq. (F2) with

$$\int_{-1}^{1} d\mu\, \mu^{-1} \int_{0}^{E_B - 3T} dE \quad ,$$

make use of the relation

$$\frac{1}{2\pi} \int_{-1}^{1} d\mu \int_{0}^{2\pi} d\varphi' \delta(\hat{v}\cdot\hat{v}' - g(E',E)) = 1 , \tag{F5}$$

and recall the definition of the total cross section from Eq. (15)

$$N\sigma^{T}(E) = \int_{E/\beta}^{E} dE' \mathcal{F}(E,E') , \tag{F6}$$

we find

$$\frac{dj(x)}{dx} - \int_{-1}^{1} d\mu\,\mu^{-1} \int_{0}^{E_B - 3T} dE \frac{\partial}{\partial E}(S(E)\Phi(E,x,\mu))$$
$$- \int_{0}^{E_B - 3T} dE \int_{E}^{\beta E} dE' \int_{-1}^{1} d\mu' \mu'^{-1} \mathcal{F}(E',E)\Psi_2(E',x,\mu') = 0 . \tag{F7}$$

We find therefore that

$$\frac{d\sigma(x)}{dx} = - \int_{-1}^{1} d\mu\,\mu^{-1} \int_{0}^{E_B - 3T} dE \frac{\partial}{\partial E}(S(E)\Phi(E,x,\mu)) . \tag{F8}$$

We expand Φ in Legendre polynomials

$$\phi(E,x,\mu) = \mu \sum_{\ell} \frac{2\ell+1}{2} \varphi_{\ell}(E,x) P_{\ell}(\mu) , \tag{F9}$$

and find that

$$\begin{aligned} \frac{d\sigma(x)}{dx} &= - \int_{0}^{E_B - 3T} dE \frac{\partial}{\partial E} (S(E)\varphi_{0}(E,x)) \\ &= S(0)\varphi_{0}(0,x) \end{aligned} \tag{F10}$$

since φ vanishes for $E = E_B - 3T$. The Hermite polynomial expansion gives

$$\frac{d\sigma(x)}{dx} = S(0) \exp\left[- \left(\frac{x - \overline{x}(0)}{\xi(0)} \right)^2 \right] \sum_{n=0}^{\infty} h_n^{-1} H_n \left(\frac{x - \overline{x}(0)}{\xi(0)} \right) \varphi_{n,0}(0) \tag{F11}$$

It is clear that without inelastic losses, there would be no stopped ions - any ion whose energy falls below T would have no mechanism for further energy loss and would never come to a stop.

Moments of the range distributions are easily calculated,

$$\begin{aligned} R_m &= \int_{-\infty}^{\infty} dx\, x^m \frac{d\sigma(x)}{dx} \\ &= S(0) \sum_{n=0}^{m} C_{n,m}(0) \varphi_{n,0}(0) \end{aligned} \tag{F12}$$

where

$$C_{n,m}(E) = h_n^{-1} \int_{-\infty}^{\infty} dx\, x^m H_n \left(\frac{x - \overline{x}(E)}{\xi(E)} \right) \exp\left[- \left(\frac{x - \overline{x}(E)}{\xi(E)} \right)^2 \right] . \tag{F13}$$

Using the recurrence relations for Hermite polynomials

$$2yH_n(y) = H_{n+1}(y) + 2nH_{n-1}(y) , \tag{F14}$$

and recalling that

$$h_n = \sqrt{\pi}\, 2^n n! \quad , \tag{F15}$$

we arrive at a recurrence relation for the $C_{n,m}$. If we let

$$C_{n,m}(E) = \xi(E)\, \hat{C}_{n,m}(E) , \tag{F16}$$

then

$$\hat{C}_{n,m} = \bar{x}(E)\, \hat{C}_{n,m-1} + (n+1)\xi(E)\, \hat{C}_{n+1,m+1}(E) + \tfrac{1}{2}\xi(E)(1-\delta_{no})\, \hat{C}_{n-1,m-1}(E) . \tag{F17}$$

If we note that

$$\hat{C}_{o,o} = 1 \text{ and } \hat{C}_{n,m} = 0, \ m < n \tag{F18}$$

we can calculate all the $C_{n,m}(E)$.

2. Energy Deposition

The energy current $\eta(x)$ is given by

$$\eta(x) = \int_{-1}^{1} d\mu \int_{o}^{E_B} dE\, E\Psi(E,x,\mu) . \tag{F19}$$

If we define $\chi(E,x)$ by

$$\chi(E,x) = \int_{-1}^{1} d\mu\, \mu^{-1}\, \Psi(E,x,\mu) , \tag{F20}$$

then the Boltzmann equation yields, after a little manipulation

$$\frac{d\eta(x)}{dx} + \int_0^{E_B} dE\, T(E)\chi(E,x) + \int_0^{E_B} dE\, S(E)\chi(E,x) = E_B\delta(x) , \tag{F21}$$

where

$$T(E) = \int_{E/\beta}^{E} dE'(E-E')\mathcal{F}(E,E') . \tag{F22}$$

We thus can identify the quantity

$$\frac{d\mathcal{E}(x)}{dx} = \int_0^{E_B} dE(T(E) + S(E))\chi(E,x) \tag{F23}$$

as the depth rate of energy deposition. The contribution from elastic and inelastic collisions are clearly separated. Using Eq. (10) from the main body of the text, we have

$$\frac{d\mathcal{E}(x)}{dx} = \left[T(E_B) + S(E_B)\right]\psi_0(x) + \int_0^{E_B} dE\, \frac{T(E)+S(E)}{g(E_B,E)}\,\psi_1(E,x)$$

$$+ \int_0^{E} dE\left[T(E)+S(E)\right]\exp\left[-\left(\frac{x-\bar{x}(E)}{\xi(E)}\right)^2\right]\sum_{n=0}^{\infty} h_n^{-1} H_n\left(\frac{x-\bar{x}(E)}{\xi(E)}\right)\left[\varphi_{n,0}(E)\right.$$

$$\left. + \Psi_{2;n,0}(E)\right] . \tag{F24}$$

The moments of the energy distribution are given by

$$V_s = \int_{-\infty}^{\infty} dx\, x^s \frac{d\mathcal{E}(x)}{dx}$$

$$= \left[T(E_B) + S(E_B)\right]A_s + \int_{E_B/\beta}^{E_B} dE\, \frac{T(E) + S(E)}{g(E_B,E)}\, B_s(E) \tag{F25}$$

$$+ \sum_{n=0}^{s} \int_0^{E_B} dE\left[T(E) + S(E)\right]C_{n,s}(E)\left[\Psi_{2;n,0}(E) + \varphi_{n,0}(E)\right], \tag{F26}$$

where

$$A_s = \int_{-\infty}^{\infty} d\,x\; x^s \psi_0(x)\,,\quad B_s(E) = \int_{-\infty}^{\infty} d\,x\; x^s \psi_1(E,x)\,. \tag{F27}$$

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